# 2,4,5-Trifluoro-3-methoxybenzoic acid, cyclohexyl ester

**Inchi:** InChI=1S/C14H15F3O3/c1-19-13-11(16)9(7-10(15)12(13)17)14(18)20-8-5-3-2-4-6-8/h7-8

**InchiKey:** WAYLDBHJMAOIIS-UHFFFAOYSA-N

**Formula:** C14H15F3O3

**SMILES:** COc1c(F)c(F)cc(C(=O)OC2CCCCC2)c1F

**Mol. weight [g/mol]:** 288.26

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -758.01 | kJ/mol | Joback Method |
| hf | -1052.67 | kJ/mol | Joback Method |
| hfus | 29.55 | kJ/mol | Joback Method |
| hvap | 61.23 | kJ/mol | Joback Method |
| log10ws | -4.93 | | Crippen Method |
| logp | 3.602 | | Crippen Method |
| mcvol | 192.120 | ml/mol | McGowan Method |
| pc | 2081.22 | kPa | Joback Method |
| rinpol | 1810.00 | | NIST Webbook |
| rinpol | 1810.00 | | NIST Webbook |
| tb | 682.39 | K | Joback Method |
| tc | 888.88 | K | Joback Method |
| tf | 427.58 | K | Joback Method |
| vc | 0.741 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 535.29 | J/mol×K | 682.39 | Joback Method |
| cpg | 551.05 | J/mol×K | 716.80 | Joback Method |
| cpg | 565.82 | J/mol×K | 751.22 | Joback Method |
| cpg | 579.61 | J/mol×K | 785.63 | Joback Method |
| cpg | 592.42 | J/mol×K | 820.05 | Joback Method |
| cpg | 604.23 | J/mol×K | 854.46 | Joback Method |
| cpg | 615.06 | J/mol×K | 888.88 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U357610&Units=SI |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |